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FINAL REPORT
ON THE MICROMECHANIC THEORY OF CONSTITUTIVE RELATIONS OF POLYCRYSTALLINE SOLIDS

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Final Report on the Micromechanic Theory of Constitutive Relations of Polycrystalline Solids

Abstract

This research is to derive the macroscopic multi-axial stress-strain and stress-strain-time relations of metals from those of the component crystals. Since the macroscopic stress-strain relation depends on the grain size, the component crystal properties are also dependent on grain size. Hence the component crystal stress-strain relation is here derived from the uniaxial polycrystal tests. This automatically takes care of the grain size effect. The same approach is used to derive the macroscopic stress-strain-time relation (creep) of metals. In this derivation, the conditions of mechanics i.e., the condition of equilibrium, and the continuity of displacement are fully satisfied. Hence the discrepancy between the calculated and experimental results is likely due to the error in representation of the component crystal characteristics. Recently Bassani (1990) and Wu et. al., (1990) have compressed a single crystal to activate a primary slip system, unloaded this crystal, then reoriented and compressed to activate a second slip system. He found the critical shear stress of the second system increases rapidly, i.e., high rate of hardening. This characteristic is not shown in a single crystal under a tensile loading. In the previous physical theories, the stress-strain relations of the component crystals were calculated from the polycrystal tensile test data (Lin, 1971) and this high hardening rate was not encountered. In the present study, this high hardening rate is considered. It is found that the agreement between the calculated and experimental results is much further improved.

Creep test are generally performed under constant stress. To apply these test data to structures under varying stress, the so called mechanical equation of state is assumed. This gives a relation between the macroscopic creep rate, stress and current creep strain under constant temperature. This relation has been found to hold approximately for tests under uniaxial tension (Lin 1968). To generalize this relation to multi-axial loading. The critical shear stress in a slip system in a crystal

to slide, is assumed to be a function of the resolved shear stress and the amounts of slip in all slip systems in the crystal. A form of this function has been found to give a good representation of the creep data under non-radial loadings given by L. Ding, 1990. The calculated and the experimental results are presented. The agreement between the present model and the experiments are much better than those calculated by Von Mise's criterion commonly used in industries.

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I. Introduction

Ductile materials can withstand much additional strain beyond their elastic range. This strain often induces a redistribution of stresses, which result in a considerable additional load-carrying capacity. To determine this load-carrying capacity, an elastic-plastic multi-axial stress-strain relation is needed. Similarly, structures subject to creep strains, we need the stress-strain-time relations. These stress-strain and stress-strain-time relations are called the constitutive relations of materials. There are six stress components and six strain components. If the stresses are proportionally increased, it is called a radial loading. If the ratios of the stress components change, it is called a non-radial loading. Many structural problems involve non-radial loadings. Plasticity and creep theories based on Von Mise's and Tresca's criteria, commonly used in industry, represent the stress-strain relation and the stress-strain-time relations reasonably well under radial loadings but show large discrepancies with experiments under non-radial loadings (Budiansky et. al., 1951).

Studies of this stress-strain relation of polycrystalline metals are generally divided into two classes. One is known as the mathematical theory of plasticity, which is mainly a representation of experimental data and does not inquire deeply into the physical basis. This type of theory using Von Mise's criterion is referred to as Mise's theory of plasticity. It does not represent well the stress-strain relation under many non-radial loadings. This theory gives an initial elastic shear modulus after the material is compressed beyond the elastic limit (Handleman and Prager 1948), and predicts an elastic-plastic buckling compressive strength of rectangular plates much higher than the experimental value. Hence this type of theory is not quite satisfactory. The other class of plasticity theory is known as the physical theory, which does attempt to explain why things happen the way they do, but may not embody mathematical simplicity. With the rapid advances of computer, the more complex mathematical representation of the physical theory is now possible for use in design and analyses.

Structures subject to loads at elevated temperatures have been greatly increased during the last few decades. At these temperatures, creep strain becomes significant and induces a redistribution of stress in redundant structures. These redistributed stresses govern the creep rates and hence the life of the structure. To analyze this stress redistribution in the structure at different time instants, a realistic stress-strain-time relation of the material is needed. The stress-strain-time relation given by "time hardening" and "strain-hardening" (Johnson and Henderson, 1962) commonly used for structural analysis often have large discrepancies with experimental results. These creep theories do not consider the physical mechanism of deformation. This seems to be one main source of error of these theories. As Dorn and Mote, 1963, have indicated, among the different mechanisms of plastic deformation, slip is the main mechanism for face-centered cubic metals at low and intermediate temperatures. Conrad, 1961 has also stated that at these temperatures, the deformation of a f.c.c. polycrystalline metal occurs essentially by deformation of the grains. Grain boundary sliding is only significant when the temperature approaches one half the melting temperature of the metal. Present study is mainly concerned with such metals and alloys at low and intermediate temperatures, hence slip is considered to be the sole source of creep deformation.

Single crystal test at room temperature (Taylor and Elam, 1923, 1925, Taylor, 1928), have shown that under stress, slip occurs along certain crystal directions on certain crystal planes. In a face-centered-cubic crystal, there are four such planes, on each of which there are three slip directions giving twelve slip systems. These planes correspond to dislocation glide planes and these directions correspond to Burgers vectors of dislocations. From dislocation theory, (Read, 1953), the force to move a segment of dislocation line is directly proportional to the shear stress on the slip plane along the Burgers vector. This is shown in single crystal tests that slip depends on the resolved shear stress along the slip direction on the slip plane and is independent of the normal pressure on the plane, Taylor, 1938. The quantitative relations between plastic strain and dislocation movement have been elegantly given by Mura, 1967, Kröner, 1958 and others. Tests on aluminum single crystals by Johnson et al., 1953, 1955, show that deformation at elevated temperatures occurred by

slip in primarily the twelve slip systems that are operative at room temperature. There also may be some slip on (311), (211) or (100) planes but their contribution is small and requires higher resolved shear stresses than that for slip in the twelve slip systems. Hence in the present study, each crystal is considered to have time dependent slip only in these twelve systems, and the rate of slip is taken to depend on the resolved shear stress, Johnson et al., 1953, 1955.

Physical theory involves two parts: one is the derivation of polycrystal stress-strain relation and stress-strain-time relation from those of the component crystal and the other is a realistic representation of the characteristics of the component crystal. These two parts are presently shown.

II. Some Previous Physical Theories of Plasticity and Creep

The main difference of a polycrystal from a single crystal is the presence of grain boundaries. The grain boundary has been estimated to be only a few atoms thick, (Dorn, and Mote, 1963, Barrett, 1952). Hence, in the calculation of slip field of a polycrystal, the grain boundary can be regarded as a surface of zero thickness across which crystal orientation changes from one to another. The anisotropy of elastic constants of single crystals varies from one metal to another. This anisotropy is small for aluminum, Barrett 1952. The present study concerns mainly with aluminum and its alloys, hence this anisotropy is neglected. When an aggregate of randomly oriented crystals of homogeneous and isotropic elastic constants is uniformly loaded, the stress is uniform throughout before slip occurs. However, crystals of different orientations have different resolved shear stresses. Assume that a crystal deforms by slip only when the resolved shear stress in some slip system exceeds certain critical value (Schwope et al., 1952). Slip occurs in the aggregate when the resolved shear stress in the most favorably oriented crystal reaches the critical value.

After the relation between the stress and strain was experimentally obtained for single crystals, many attempts were made to reduce the stress-strain relation of the polycrystal from the single crystal data. The first pioneering realistic model was proposed by Taylor, 1938. He assumed all crystals to be rigid-plastic. His neglect of elastic strain causes significant error when the elastic

and plastic strains are of the same magnitude. Lin, 1957, modified Taylor's model to include elastic strain. However, both Taylor's model and this model of Lin's satisfy the condition of compatibility but not that of equilibrium across the grain boundaries. A rigorous model satisfying both these conditions was given by Lin (1971) and is described in a later section. Recently, Tokuda, Kratochvil and Ohasi (1981) applying this Lin's model to a two dimensional polycrystal, calculated the variation of the macroscopic stresses under some arbitrary strain paths and have found their calculated values agreeing fairly well with experimental results.

Batdorf and Budiansky, 1949 proposed a simplified slip theory assuming each component crystal in a aggregate to subject to the same stress and slide in slip systems, independent of other crystals. This theory and some other theories satisfy the condition of equilibrium but not compatibility.

Eshelby in 1957 has shown that an ellipsoidal inclusion in an infinite homogeneous elastic medium to undergo a change in shape and size that would be an arbitrary homogeneous strain if the surrounding material were absent, will cause a uniform strain inside the inclusion. Based on this result, Kröner (1961) considered each crystal in a uniformly loaded polycrystals as an ellipsoidal inclusion in a homogeneous infinite elastic medium. The crystal orientations are assumed to be randomly distributed in the aggregate. The sum of the loads carried by all the individual crystals cut by a section must balance the applied load. The stress relieved by slid crystals must be carried by other crystals. Hence the sliding of one group of crystals increases the average load taken by other groups of crystals. Kröner took this average interaction effect between groups of crystals into consideration and developed an analytical procedure to calculate the polycrystal stress-strain relationship from single crystal characteristics. Budiansky and Wu (1962) rederived Kröner's scheme by a different physical reasoning. This scheme is called the self-consistent method for polycrystal plasticity analysis. When slip has occurred in a significant portion of the aggregate, the matrix of the inclusion has pronounced directional weakness. A theory taking into consideration this directional weakness has been proposed by Hershey (1957) and Hill (1965). Hutchinson (1970)

using Hill's model, calculated the incremental stress-strain relations at different ratios of incremental shear and compressive-stresses after the metal is stressed in compression beyond the elastic range. Studies by this self-consistent method have contributed a great deal to the understanding of the plastic deformation of polycrystals.

In this self-consistent approach, each crystal is considered as an inclusion in the calculation of the amount of slip in the crystal and is also considered as part of the matrix when the slip is calculated for any other crystal. The stress in a crystal should be the sum of the stress as an inclusion and as part of the matrix. However, the stress as in the role of matrix is not explicitly considered in the calculation of slip. The stress caused by one slid crystal on another increases rapidly as the distance between these two crystals is decreased. The average interaction effect of slid crystals provided by the self-consistent theory does not consider the distance between the slid crystals. Slip and slip rate vary nonlinearly with the resolved shear stress. This nonlinear effect introduces errors in using this average interaction effect in calculating the macroscopic plastic strain. In most numerical calculations of the approach, spherical inclusions were considered. The resolved shear stress $\Delta\tau$ relieved in such an inclusion is $2\nu(1-b)e''_{\alpha\beta}$ where $b = 2(4-5\nu)/15(1-\nu)$. With μ denoting shear modulus; ν Poisson's ratio and $e''_{\alpha\beta}$ the plastic resolved shear strain along the slip direction β on the slip plane with normal α, this $\Delta\tau$ with $\nu = 0.3$ gives an $\Delta\tau = .524 \times 2\mu e''_{\alpha\beta}$. The plastic strain distribution in an inclusion of cubic shape to relieve a constant resolved shear stress was calculated by Lin et. al., (1961). The average plastic strain in this inclusion to relieve 0.1 C_o stress is about $.14\ C_o/2\mu$. This gives $\Delta\tau = .71 \times 2\mu e''_{\alpha\beta}$. Hence spherical inclusions are softer than cubic inclusions. From the micrographs of the grain boundaries, the crystals in the aggregate are of polygonal shape. Besides, three-dimensional space cannot be filled by ellipsoids alone. The assumption of all crystals to be spherical is not realistic.

Assuming the rate of slip in a slip system to be governed by the resolved shear stress in that system, Rice, 1970, has shown that it is possible to derive the polycrystal macroscopic creep strain rate from a potential function of stress. Phillips, 1969, has experimentally obtained loading surfaces

of polycrystal aluminum under combined loading at elevated temperatures. Brown, 1970a, b, has extended the application of the Budiansky-Wu's self-consistent model of plastic deformation to creep strains. Assuming the slip rate $\dot{\gamma}$ in a slip system to be a power function of the resolved shear stress τ in that system,

$$\dot{\gamma} = c\tau^n$$

where c and n are constants and n varies from 3 to 8, Brown has calculated, by this self-consistent model, the creep strain rates under a given path of non-radial loading. He has compared the calculated results with experimental strain-rate vs time curves and has found that the experimental curves gives much larger creep strain rate than the calculated results following each change in loading. Hutchinson, 1975, has shown a more direct method of estimating the steady creep characteristics of polycrystals composed of f.c.c. crystals whose slip rate in a slip system is a power function of its resolved shear stress. These studies have contributed much to the understanding of the relation between the creep properties of single crystals and those of polycrystals.

When a polycrystal is loaded at an elevated temperature, many or all crystals may slide; then the distance between two adjacent slid crystals may become very small. Hence the application of Eshelby's results considering the average interaction effect may cause significant error. The assumption of creep rate of a single crystal as a function of the resolved shear stress only, neglects the transient creep. This neglect of transient creep and the use of the self-consistent theory seem to be the main cause of the discrepancy between Brown's calculated and experimental results (Brown, 1970a, b).

III. Derivation of Polycrystal Stress-Strain and Stress-Strain-Time Relations From those of the Component Crystal

Many metals undergo considerable plastic deformation without crack, so crystals originally in contact remain so during deformation. This means that equilibrium and continuity of displacement are satisfied throughout the aggregate. But the previous models do not simultaneously satisfy both

the equilibrium and compatibility conditions.

A. Analogy of Inelastic Stress and Applied Forces

In order to have the aggregate stress and strain fields fully satisfying both the equilibrium and compatibility conditions, Lin et. al., (Lin and Ito 1966, Lin 1971) have generalized Duhamel's analogy of thermal strain to include plastic strain. Neglecting the anisotropy of elastic constants and considering the plastic strain to have no dilatation, the stress-strain relations are then

$$\tau_{ij} = \delta_{ij}\lambda e_{kk} + 2\mu(e_{ij} - e''_{ij}) \tag{1}$$

where λ and μ are Lame's constants and δ_{ij} is Kronecker delta. Substituting (1) into the equations of equilibrium yields

$$\delta_{ij}\lambda e_{kk,j} + 2\mu e_{ij,j} - 2\mu e''_{ij,j} + F_i = 0 \tag{2}$$

and

$$S_i^{\nu} = [\lambda e_{kk} + 2\mu(e_{ij} - e''_{ij})]\nu_j \tag{3}$$

where F_i is the body force per unit volume, S_i^{ν} the surface force along the i-axis per unit area with the normal $\underline{\nu}$. The subscript j after comma denotes differentiation along the j-axis. The repetition of the subscript "j" denotes summation from one to three. It is seen that $-2\mu e''_{ij,j}$, is equivalent to F_i and $2\mu e''_{ij}\nu_j$ to S_i^{ν} in causing the strain field e_{ij} and hence are called the equivalent body force $\overline{F}_i$ and surface force $\overline{S}_i^{\nu}$ respectively. Denoting the stress caused by $\overline{F}_i$ and $\overline{S}_i^{\nu}$ by τ_{ij}^{s}, the residual stress caused by the plastic strain is given by Eq. 1 as,

$$\tau_{ij}^{R} = \tau_{ij}^{s} - 2\mu e''_{ij} \tag{4}$$

With this analogy, the solution of the stress and strain fields of an aggregate with plastic and/or creep strain reduces to the solution of stress and strain fields caused by a given force applied to a 3-dimensional elastic body. This analogy gives the same results as those obtained by Eshelby's

ingenious process of imaginary cutting, welding, relaxing etc. in his paper on ellipsoidal inclusions in 1957. Hence the present method developed by Lin et. al., satisfies both equilibrium and compatibility conditions.

B. An Aggregate in an Infinite Elastic Medium: (Lin, 1984)

To solve a 3-dimensional elasticity problem with a given set of boundary conditions is a big task. To avoid this task we consider this aggregate to be embedded in an infinite elastic solid of the same elastic constants. Hence the equivalent body force due to plastic strain is considered to be applied in an infinite elastic medium. This aggregate is considered to consist of a large 3-dimensional solid composing of innumerous basic cubic blocks. Each block with side "*a*" consists of 64 differently oriented cube-shaped crystals. The average stress and plastic strain of the center block represent the macroscopic stress and strain of the polycrystal. The use of innumerous cubic blocks surrounding the center block is to make the center block to deform more easily than just to embed it in an elastic medium.

We consider slip occurring at $\underset{\sim}{x}'$ in the *n*th slip system causing a plastic strain $e''\left(\underset{\sim}{x}', n\right)$ [Lin, 1971]. This *n*th system has a sliding plane with normal α and a slip direction β, then the plastic strain

$$e''_{ij}(x') = \frac{1}{2} L^n_{ij} e''(x', n) \tag{5}$$

where

$$L^n_{ij} = (\alpha^n_i \beta^n_j + \alpha^n_j \beta^n_i) \tag{6}$$

The equivalent body force

$$\overline{F}_k = -2\mu \frac{\partial e''\left(\underset{-}{x}',n\right)}{\partial x_l'} \; L_{kl}^n \tag{7}$$

Kelvin's Solution of an Infinite Elastic Medium:

The displacement fields in this infinite elastic solid caused by this body force acting in a volume dV' has been given by Kelvin (Love 1927). His solution gives a stress field caused by F_k as

$$\begin{aligned} \tau_{ij}^r(x) &= \int_{v'} \phi_{ijk}\left(\underset{-}{x},\underset{-}{x}'\right) F_k\left(\underset{-}{x}'\right) \; dV' \\ &= -2\mu \int_{v'} \phi_{ijk}\left(\underset{-}{x},\underset{-}{x}'\right) \left[\frac{\partial e''\left(\underset{-}{x}',n\right)}{\partial x_l'} L_{kl}^n \right] \; dV' \end{aligned} \tag{8}$$

where $\phi_{ijk}(x,x') = - \dfrac{3}{8\pi(1-\nu)} \dfrac{(x_i - x_i')(x_j - x_j')(x_k - x_k')}{r^5}$

$$+ \frac{1-2\nu}{8\pi(1-\nu)} \left[\frac{\delta_{ij}(x_k - x_k') - \delta_{ik}(x_j - x_j') - \delta_{jk}(x_i - x_i')}{r^3} \right]$$

$$r^2 = (x_i - x_i')(x_i - x_i')$$

The size of the 3-dimensional solid may be considered as being infinite as compared to the size of one block, so the variation of plastic strain from one block to another in the center of this solid is small and neglected. The slip distributions in the blocks around the center block are taken to be the same. Hence to calcualte the stress in the center block, the values of the incremental plastic strain $\Delta e''\left(\underset{-}{x}',n\right)$ and its gradient $\partial \Delta e''\left(\underset{-}{x}',n\right)/\partial x_l'$ at (x_1', x_2', x_3') are taken to be the same as those at any point $(x_1' - m_1 a, x_2' - m_2 a, x_3' - m_3 a)$, where m_1, m_2, m_3 are any integer. Then the integral (8) over the 3-dimensional infinite region reduces to an integral over one basic block with $\phi_{ijk}\left(\underset{-}{x},\underset{-}{x}'\right)$ expressed as $\phi_{ijk}(x_1, x_2, x_3, x_1' - m_1 a, x_2' - m_2 a, x_3' - m_3 a)$ with m_1, m_2, m_3 summed over all integers.

C. Virtual Work Condition: (Wu, 1989)

Let T_{ij} and δE_{ij} be the macroscopic stress and virtual strain of the aggregate. The virtual work of the aggregate is then

$$\delta W = T_{ij}\delta E_{ij}$$

Let $\Delta\tau_{ij} = \tau_{ij} - \bar{\tau}_{ij}$ and $\Delta e_{ij} = e_{ij} - \bar{e}_{ij}$, where τ_{ij} and e_{ij} denotes the microscopic stress and virtual strain respectively and bar on top denotes the average value. The

$$\begin{aligned}\delta W &= \int_V \tau_{ij}\delta e_{ij}dV = \int_V (\bar{\tau}_{ij} + \Delta\tau_{ij})(\delta\bar{e}_{ij} + \delta\Delta e_{ij})dV \\ &= \int_V \bar{\tau}_{ij}\delta\bar{e}_{ij}dV + \int_V \Delta\tau_{ij}\delta\Delta e_{ij}dV \qquad (9)\end{aligned}$$

Since the average stress and strain in the block are taken to represent its macroscopic stress and strain, the virtual work per unit volume,

$$\delta W = T_{ij}\delta E_{ij} = \bar{\tau}_{ij}\delta\bar{e}_{ij} + \frac{1}{V}\int_{\Gamma} \Delta\tau_{ij}n_j\delta\Delta u_i dV \qquad (10)$$

Let the displacement u_i be expressed as

$$u_i = \bar{u}_i + \Delta u_i$$

To satisfy the compatibility condition, the displacement on the two opposite planes (normal to j-axis) of the basic block with a linear dimension "a" must satisfy the condition

$$\delta\Delta u_i|_{\Gamma_j\left(\frac{a}{2}\right)} = \delta\Delta u_i|_{\Gamma_j\left(\frac{-a}{2}\right)}$$

To satisfy the equilibrium condition, we have

$$\Delta\tau_{ij}n_j|_{\Gamma_j(a)} = \Delta\tau_{ij}n_j|_{\Gamma_j(-a)} \qquad \text{no summation on } j$$

Hence the second term on the right-hand side of (10) vanishes (Wu, 1989).

$$T_{ij}\delta E_{ij} = \bar{\tau}_{ij}\delta\bar{e}_{ij} \tag{11}$$

For an incremental loading, let ΔT_{ij} be the incremental macroscopic stress and $\Delta E'_{ij}$ be the incremental elastic macroscopic strain.

$$\Delta E'_{ij} = M_{ijkl}\Delta T_{kl} = M_{ijkl}\Delta\bar{\tau}_{ij} = \Delta\bar{e}'_{ij} \tag{12}$$

where M_{ijkl} is the elastic compliance, $\Delta E_{ij} = \Delta E'_{ij} + \Delta E''_{ij} = \Delta\bar{e}'_{ij} + \Delta\bar{e}''_{ij}$. Hence $\Delta E''_{ij} = \Delta\bar{e}''_{ij}$. This gives

$$T_{ij}\delta E''_{ij} = \bar{\tau}_{ij}\delta\bar{e}''_{ij} \tag{13}$$

Bishop and Hill (1951), Hill (1963, 1967) have shown that this virtual work equation for polycrystal aggregate is valid only when either the tractions or the displacements on the boundaries are uniform. In the present model, this relation holds even neither the traction nor the displacement on the boundaries of the block is uniform.

D. Crystal Orientations:

Metals generally are composed of crystals of random orientations. Their macroscopic stress T_{ij} and plastic strain E''_{ij} generally satisfy the condition $E''_{22} = E''_{33} = -\frac{1}{2}E''_{11}$, $E''_{12} = E''_{23} = E''_{31} = 0$ under tensile loading T_{11}. Similar conditions have been observed under loading T_{22} or T_{33}. Under a pure shear loading $T_{ij}(i \neq j)$, all plastic strain components except E''_{ij} vanish. These properties have been referred to as the initial isotropy of polycrystals. In order to simulate this property, the 64 crystals in the basic block are divided into 8 groups, each of which occupies one octant. Among the 8 crystals in the first octant, one crystal has a slip system most favorable under uniaxial loading

T_{11} and another under T_{12}. If the T_{12} to initiate slip is 0.50 or 0.577 of T_{11} in initiating slip, this gives Tresca's or Von Mise's criterion for initial yielding. Another crystal is oriented to give a mirror image of the first with respect to the plane making 45° with x_2 and x_3 axes. These give two crystals associated with T_{11}. Similarly, there are two crystals associated with T_{22} and two with T_{33}. These take 6 crystals. The remaining two crystals have their axes coinciding with the specimen axes. The positions of these 8 crystals are chosen so as to give no preference to loading T_{11}, T_{22} or T_{33}. As for the other seven groups of crystals, the orientations and arrangement of each group are chosen to give mirror images to other groups with respect to the three coordinate planes of the specimen axes. This gives three planes of symmetry and satisfies the property of cubic symmetry. By this way, the property of initial isotropy of polycrystals, referring to this set of axes, is fulfilled.

E. Simplification of Numerical Calculation: (Lin and Ribeiro, 1981)

To simplify the numerical calculation, the plastic strain is assumed to be uniform in each crystal. Then plastic strain gradient within each crystal vanishes, but across the boundary, plastic strain drops from the uniform value to zero and causes an equivalent uniform surface force on the plane boundary surfaces. The stress-field at x caused by this surface forces due to slip in the nth slip system of the qth crystal is obtained by integrating Eq. 8 as

$$\tau_{ijqn}\left(\underset{\sim}{x}\right) = 2\mu \oint \sum_{m_1}\sum_{m_2}\sum_{m_3} \phi_{ijk}\left(\underset{\sim}{x}, \underset{\sim}{x}', m_1, m_2, m_3\right) e''(q,n) L^n_{kl}(q)\, d\Gamma_l \tag{14}$$

integrated over the boundary surfaces of the crystal, where $d\Gamma_l$ denotes the differential projected boundary area on the plane normal to x_l-axis. In evaluating the infinite triple sums, the cubic blocks were grouped according to their distance from the center block. Let

$$m_1^2 + m_2^2 + m_3^2 = k^2$$

The triple sum is evaluated with monotonically increasing values of k^2. It was found that these sums converge well at $k^2 = 48$. The average stress of the pth crystal calculated from Eq. 8 is written (Lin, 1984), as

$$\tau^S_{ijqn}(p) \;=\; 2\mu e''(q,n) L^n_{kl}(q)\phi_{ijlk}(p) \tag{15}$$

The average residual stress of the sth crystal due to slip in the nth slip system of the qth crystal

$$\begin{aligned}\tau^R_{ijqn}(s) &= 2\mu[n_{kl}(q)\phi_{ijkl}(s) - \delta_{sq}L^n_{ij}(s)]e''(q,n)\\ &= a_{ijqn}(s)e''(q,n)\end{aligned} \tag{16}$$

Under a uniform stress τ^0_{ij} applied to the infinite medium.

$$\tau_{ij}(s) \;=\; \tau^0_{ij} + a_{ijqn}e''(q,n) \tag{17}$$

The average stress $\bar{\tau}_{ij}$ over the 64 crystal block represents the macroscopic stress S_{ij}. We have

$$\Delta S_{ij} \;=\; \Delta\bar{\tau}_{ij} \;=\; \Delta\bar{\tau}^0_{ij} + \bar{a}_{ijqn}\Delta e''(q,n) \tag{18}$$

where the bar denotes the average value of the 64 crystals. Writing (17) in incremental form and substituting $\Delta\tau^0_{ij}$ from (18), we have

$$\Delta\tau_{ij}(s) \;=\; \Delta S_{ij} + (a_{ijqn} - \bar{a}_{ijqn})\Delta e''(q,n) \tag{19}$$

The 2nd term represents the increase of stress due to incremental slip $\Delta e''(q,n)$. Let

$$c_{spqn} \;=\; m_{ij}(s)\,(a_{ijqn} - \bar{a}_{ijqn}) \tag{20}$$

The incremental resolved shear stress in the mth slip system of the sth crystal

$$\Delta\tau_{sm}(s) \;=\; m_{ij}(s)\Delta S_{ij} + c_{pmqn}\Delta e''(q,n) \tag{21}$$

where c_{pmqn} is the influence coefficient of the resolved shear stress in the mth slip system of the sth crystal caused by a unit plastic strain in the nth slip system of the qth crystal. The influence coefficients satisfy this reciprocal relation and form a symmetric matrix.

Let τ_{cr} denote the critical shear stress. These slip systems with resolved shear stress equal to the critical, i.e., $\tau^m = \tau_{cr}^m$ are called the potentially active systems. Those potentially active systems with $\Delta\tau^m = \Delta\tau_{cr}^m$ will slide. Hence from Eq. 21, $\Delta\tau^m = \Delta\tau_{cr}^m$ governs the amount of slip in different slip systems. There are as many such equations as the number of unknown $\Delta e''(s,m)$'s.

E. Takahashi's Verification by Finite Element Analysis:

Takahashi (1987) examined this polycrystal plasticity model by 2-dimensional finite element analysis. A two-dimensional inhomogeneous problem of a non-hardening infinite medium containing inclusions subject to a simple tension was calculated by the finite element method. The calculated results of the plastic strains were substituted in this and a self-consistant model to get the stress fields, which were compared with the results of FEM. It was found that Lin's model agrees well with the FEM, but not the self-consistent model As indicated by Takahashi, 1987, "the validity of the Lin model has been proved".

IV. Single Crystal Time-Independent Slip Characteristics

A. Taylor's Isotropic Hardening:

Early single crystal tests (Taylor 1938) have shown that under stress slip occurs along certain crystal directions on certain crystal planes. This slip depends on the resolved shear stress and is independent of its normal pressure on the sliding plane. The critical shear stress in duplex slip (two active slip systems) depends on the sum of slip in the two systems. Based on these early results, Taylor assumed the active and latent slip systems to have the same critical shear stress. This model

is known as isotropic hardening, which is a first approximation of the deformation behavior of single crystals. Based on this approximation, Taylor has calculated the stress-strain relation of the polycrystal under tension from that of single crystals.

B. Latent Hardening and Kinematic Hardening:

To refine Taylor's isotropic hardening, Wu 1989 considered two cases: (1) the single crystals to have latent hardening rates to be 1.2 to 1.4 of that of active hardening and (2) these crystals to have kinematic hardening. In the latter, the yield surface moves rigidly in stress space and gives Bauschinger effect. Using these single crystal characteristics, Wu, 1989 has derived the component crystal of the polycrystal and then calculated incremental stress-strain relations of the polycrystal loaded under different ratios of incremental shear to axial loadings, after being compressed beyond the elastic range. The calculated results are compared to the experimental results carefully obtained by Budiansky et. al., 1951. These calculated results give agreement with the experiments better than the Von Mise's and Tresca's criteria, but appreciable discrepancies were still found between the calculated and experimental results.

C. Bassani's Interpretation of Single Crystal Tests (Bassani, 1990):

Single crystal tests under tensile loading σ gives a resolved shear stress τ in the most favorably slip system. $\tau = m\sigma$, where m is the Schmid's factor. From the measured axial extension e, the shear strain γ is calculated from the expression $\gamma = e/m$. The total axial plastic strain was assumed to be due to slip in this system alone. A typical $\tau - \gamma$ curve for a f.c.c. single crystal with the tensile axis oriented within the standard sterographic triangle, is shown in Fig. 1.

Let $\dot{\gamma}_l$ denote the rate of slip on the lth slip system with unit normal n_l and slip direction s_l. The resolved shear stress in this system

$$\tau_l = L^l_{ij}\tau_{ij},$$

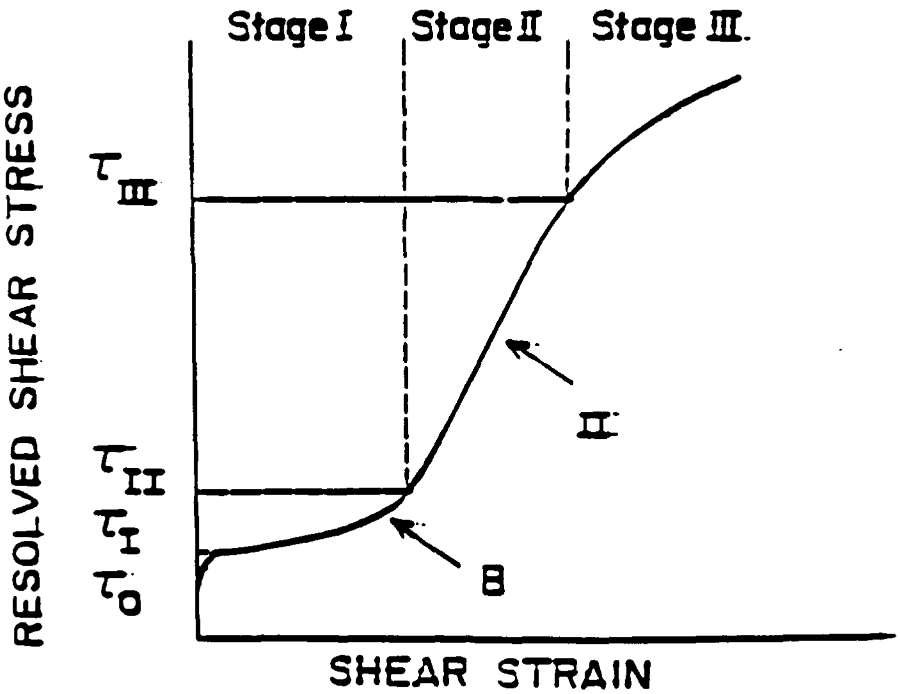


Fig. 1. **Typical $\tau-\gamma$ curve of a pure FCC single crystal loaded in uniaxial tension/compression with an initial orientation for single slip. Point B denotes where secondary slip commences and II denoted state in Stage II deformation.**

Representing the hardening rate of a slip system as a linear combination of slip rates of all systems (Hill, 1966).

$$\dot{\tau}^c_m = \sum_{n=1}^{N} h_{mn}\dot{\gamma}_n \tag{22}$$

where N denotes the total number of slid systems, h_{mn} denotes the hardening rate for the mth slip system due to slip in the nth slip system and dot denotes the time rate. In Stage I (Fig. 1), only system 1 is activated.

$$\dot{\gamma}_1 \geq 0, \qquad \dot{\gamma}_2 = 0$$

At point B of Fig. 1,

$$\tau_1^B = \tau_{o_1}^c + \int_o^{\gamma_B} h_{11} d\gamma_1 ; \qquad \tau_2^B = \tau_{o_2}^c + \int_o^{\gamma_B} h_{21} d\gamma_1 \tag{23}$$

For simplicity, assume $\tau_{o_1}^c = \tau_{o_2}^c$ and $\tau_2^B - \tau_o^c = q(\tau_1^B - \tau_o^c)$, where q is the constant. Experimental evidence indicates that at the beginning of deformation II, as indicated by B (Fig. 1) the loading axis is within the standard triangle. This indicates $m_2^B < m_1^B$. Hence $\tau_2^B/\tau_1^B = m_2^B/m_1^B < 1$. This leads to $0 < q < 1$ and $h_{21} < h_{11}$. This indicates that latent hardening is less than active hardening (Bassani 1990).

Writing Eq. 22 for incremental plastic strain, the incremental critical shear stress $\Delta\tau^c(s,m)$ in the m*th* slip system of the *s*-crystal is then

$$\Delta\tau^c(s,m) = h_{mn}(s)\Delta e''(s,n) \tag{24}$$

Equating the incremental resolved shear stress given by Eq. 21 to the above,

$$m_{ij}(s)\Delta S_{ij} + C_{pmqn}\Delta e''(q,n) = h_{mn}(s)\Delta e''(s,n) \tag{25}$$

This gives a set of linear equations. Writing in matrix form, we have the non-diagonal coefficients less than the diagonal coefficients. This facilitates much the numerical solution of the incremental slip strains. Bassani and his colleagues (Wu et. al., 1990) have further shown a single crystal test in latent hardening experiment. The crystal was first compressed to activate the primary slip system $(11\bar{1})[101]$ denoted by the subscript 1. After the plastic compression has developed to some extent, the crystal was unloaded, reoriented and reloaded to activate a secondary slip system $(\bar{1}11)[101]$ denoted by subscript 2. The compression rate was kept constant. A typical resolved shear stress and strain curve is shown in solid lines in Fig. 2. The test data had been interpreted as the dotted line giving latent hardening more than active hardening. Actually the test data is given by the solid line. At the start of reloading, the critical stress τ_1 in the primary system is larger than that in the secondary system τ_2. However right after reloading, τ_1^c seems to dip a little (Fig. 7, Wu et al, 1990)

and the hardening rate of the secondary system starts out very high and then decreases. More tests of this type are desirable. These characteristics are not represented by isotropic hardening nor well represented by a linear hardening of slip systems in different systems as given by Eq. 22. Their data seem to indicate that the hardening rates are greatly affected by the change of the ratios of the incremental slip in different systems. Let the distribution of slip rates of slip systems be represented by

$$V_m = \frac{\Delta\gamma_m}{\sum_n \Delta\gamma_n} \qquad (26)$$

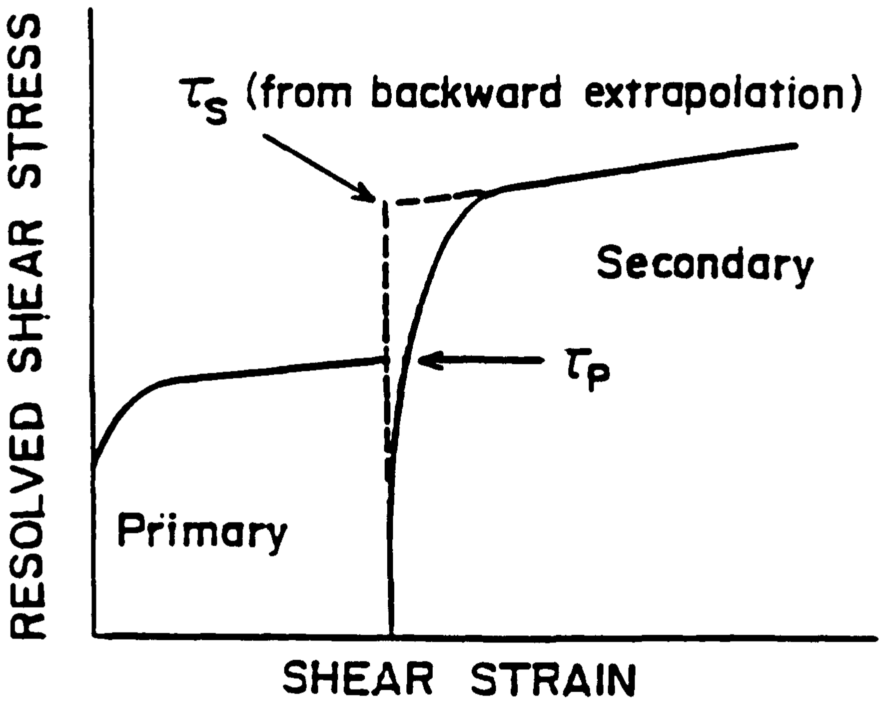


Fig. 2. $\tau-\gamma$ Curve from the Latent Hardening Experiment.

Referring to Fig. 3, the rate of compression on the specimen was constant, so the rates of slip are taken to be constant as shown by the straight lines, γ_1 from 0 to A; and γ_2 from A to B with a small γ_2 occurs before A and a small γ_1 before B.

$$V_1 = \frac{\Delta\gamma_1}{\Delta\gamma_1 + \Delta\gamma_2} \quad ; \quad V_2 = \frac{\Delta\gamma_2}{\Delta\gamma_1 + \Delta\gamma_2} \tag{27}$$

V_1, V_2 versus the summation of slip in all slip systems are plotted in Fig. 4. To represent the hardening effect due to change of slip distributions, we modify Eq. 22 by adding a term to the right-hand side giving

$$\Delta\tau^c_m = \sum_n h_{mn}\Delta\gamma_n + f[V_m, \tau^c_m] \tag{28}$$

where $f[V_m, \tau^c_m]$ has the same units as $\Delta\tau^c_m$ and represents the large increase of critical shear stress in the second slip system at the change of crystal orientation (Fig. 2). To evaluate $f[V_m, \tau^c_m]$ more closely more single crystal tests with orientation changes are needed. Considering the aggregate to have eight different oriented crystals with 12 slip systems in each crystal, we have a total of 96 slip systems. Writing Eq. 21 in a differential form with subscripts m and n denoting one of the 96 slip systems,

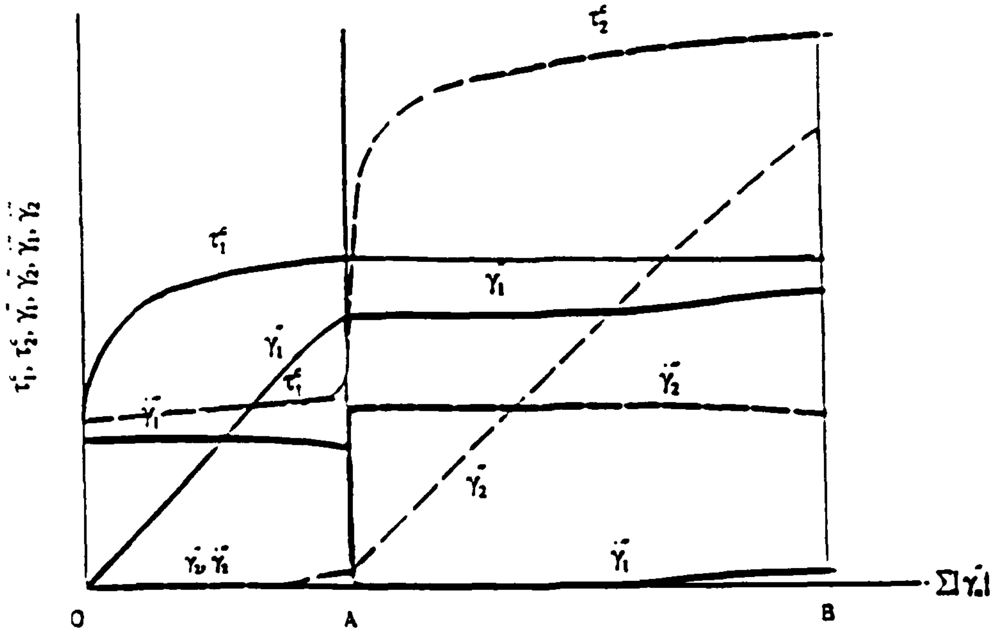


Fig. 3. Variation of Critical Shear stress τ_1, τ_2, Slip Strains γ_1, γ_2

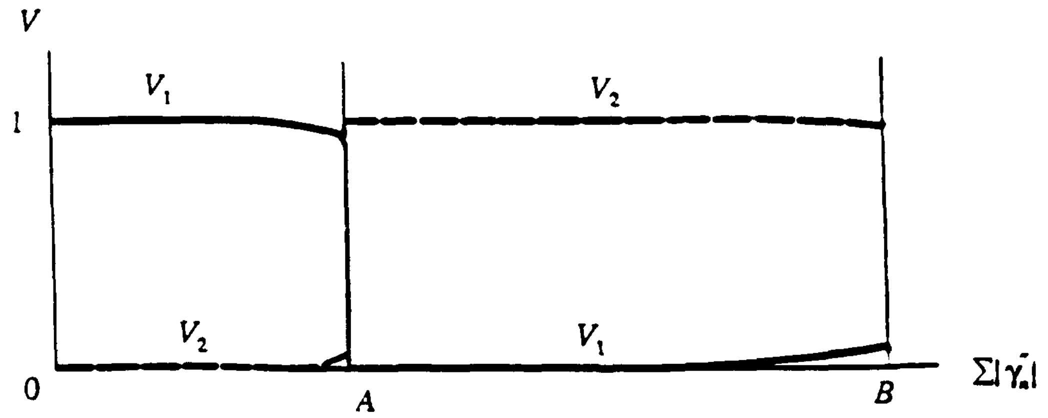


Fig. 4. Variation of V_1 V_2 in Latent Hardening Test

$$\Delta\tau_m = \Delta\tau_m^A + \sum_{n=1}^{96} C_{mn}\Delta\gamma_n \tag{29}$$

Equating this to $\Delta\tau_m^c$ in Eq. 28, gives

$$\Delta\tau_m = \Delta\tau_m^A + \sum_{n=1}^{96} C_{mn}\Delta\gamma_n = \sum_{n=1}^{12} h_{mn}\Delta\gamma_n + f(V_m, \tau_m^c) \tag{30}$$

D. Calculation of Component Crystal Stress-Strain Relation from Polycrystal Tests:

The size of single crystals in single crystal tests is much larger than that of the grains in the poly-crystal and it is known that the stress-strain curve of crystals varies with grain size (Livingston et al., 1975). Hence the component crystal stress-strain relationship is calculated from the experimental polycrystal tensile stress-strain curve (Lin, 1971). This approach is similar to the derivation of the characteristic shear function from the tensile stress-strain curve in the development of the first simplified slip theory of plasticity by Batdorf and Budiansky 1949. This is a reverse process to the calculation of polycrystal stress-strain relation from a given single crystal characteristic. In polycrystals under tensile loading, the ΔV_m's in the component crystals are small and are neglected. Eq. (28) reduces to Eq. (22). The set of h_{mn}'s were found from the tensile stress strain curve of the polycrystal. Kinematic hardening is first assumed and the variation of the critical shear stresses in

different slip systems in the component crystal are derived from the polycrystal test data. Previously, these component crystal stress-strain relations was calculated from a polycrystal tensile loading test data (Batdorf and Budiansky, 1949, Lin, 1971). In the present study, these component crystal stress-strain relation are calculated from not only from the polycrystal tensile test data, but also from the polycrystal stress-strain relation under a non-radial loading (Figs. 7 and 9). From the latter, $f(V_m, \tau_m^c)$ were found. This takes care of the effect of the change of slip distributions.

V. Numerical Calculation of Polycrystal Stress-Strain Relation

The orientation of a crystal is completely determined by the orientation of one of its slip systems. Referring to the crystals in the first octant of the cubic block (Fig. 5), the orientation of the first slip system of the crystal is defined by the normal α to the slip plane and the slip direction β as shown in Fig. 6, where θ_1 and θ_2 are taken to be 80° and 12° respectively. The orientations of the other seven crystals are determined to obtain cubic orthotropy. Crystal orientations of the other seven octants of the cubic block are obtained to give mirror images with respect to the three coordinate planes, as described in Section III.

The polycrystal considered is aluminum alloy 14ST. Its mechanical properties are:

Shear modulus G = 27,241 MPa (3.95×10^3 k.s.i.)

Poisson's ratio $\nu = 0.3$

Tensile initial yield stress 179 MPa (26 k.s.i.)

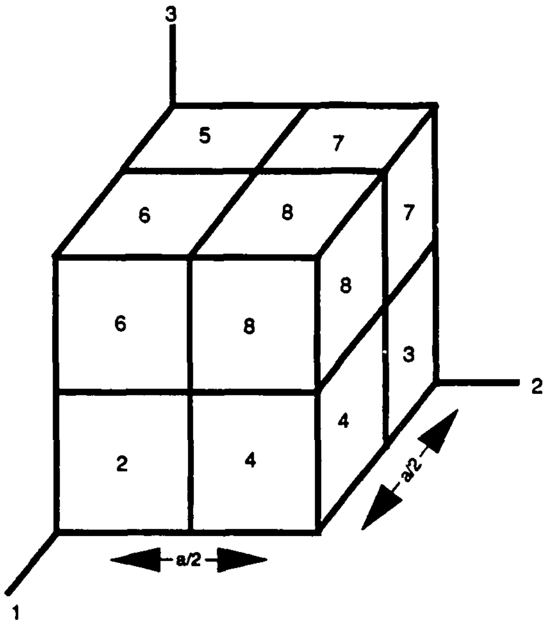


Fig. 5. Crystal Numbers in the First Octant of the Block

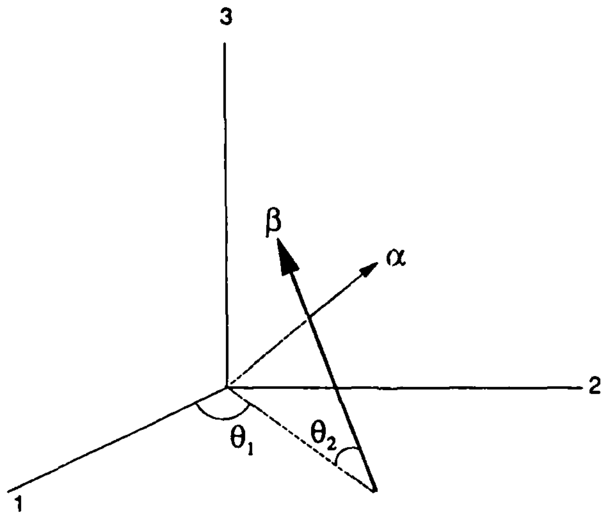


Fig. 6. Orientation of a Slip System α Normal to Slip Plane, β Along Slip Direction

Assuming kinematic hardening, the active hardening coefficient $h_{\underline{nn}}$ (no summation on "n") of the component crystal was calculated from the axial test data of the polycrystal. All the polycrystal

test data were taken from the tests performed by Budiansky et al., 1951, Fig. 7. Then $f(V_m, \tau_m^c)$ of Eq. 28 was computed from one non-radial loading, (Fig. 8) and check with another (Fig. 10). It was found the last term in Eq. 28 can be approximately represented by

$$f(V_m, \tau_m^c) = \begin{cases} C_2 \tanh\left[1.2V_m\sqrt{\dfrac{\tau_m^c}{\tau_0^c} - 1}\right] & ; \quad \dfrac{\Delta V_m}{V_m} > 0 \\ C_1(1 - V_m)^{0.2} \sqrt{\dfrac{\tau_m^c}{\tau_0^c} - 1} & ; \quad \dfrac{\Delta V_m}{V_m} \le 0 \end{cases}$$

$c_1 = 0.26, \qquad c_2 = 2.2$

$\Delta\tau^c$, c_1 and c_2 are in k.s.i.

When more single crystal data with orientation change are available. The above expression may be more accurately determined. Using the above described model with the above expression of $f(V_m, \tau_m^c)$, we have calculated the incremental stress-strain relation for the cases with the ratios of incremental axial to incremental shear stress of 1.18 and -0.652 of the specimens after being compressed beyond the elastic range. The calculated results are shown with the experimental data in Figs. 9 and 11. The comparison between Von Mise's flow theory and the experimental results are shown in the paper by Budiansky et. al, 1951. It is seen that the present theory gives a much realistic representation of the experimental results.

The above method has also been used to calculate the macroscopic plastic deformation under static tension and cyclic shear. Two cases of component crystal hardening were considered. One is isotropic hardening and the other is kinematic hardening. The growth of the polycrystal plastic axial and shear strains verses cycles of loading were calculated. The details and the numerical results are given in ASME, PVP, Vol. 184, visco-plastic behavior of new materials, Book No. H00576, pp. 79-83, 1989.

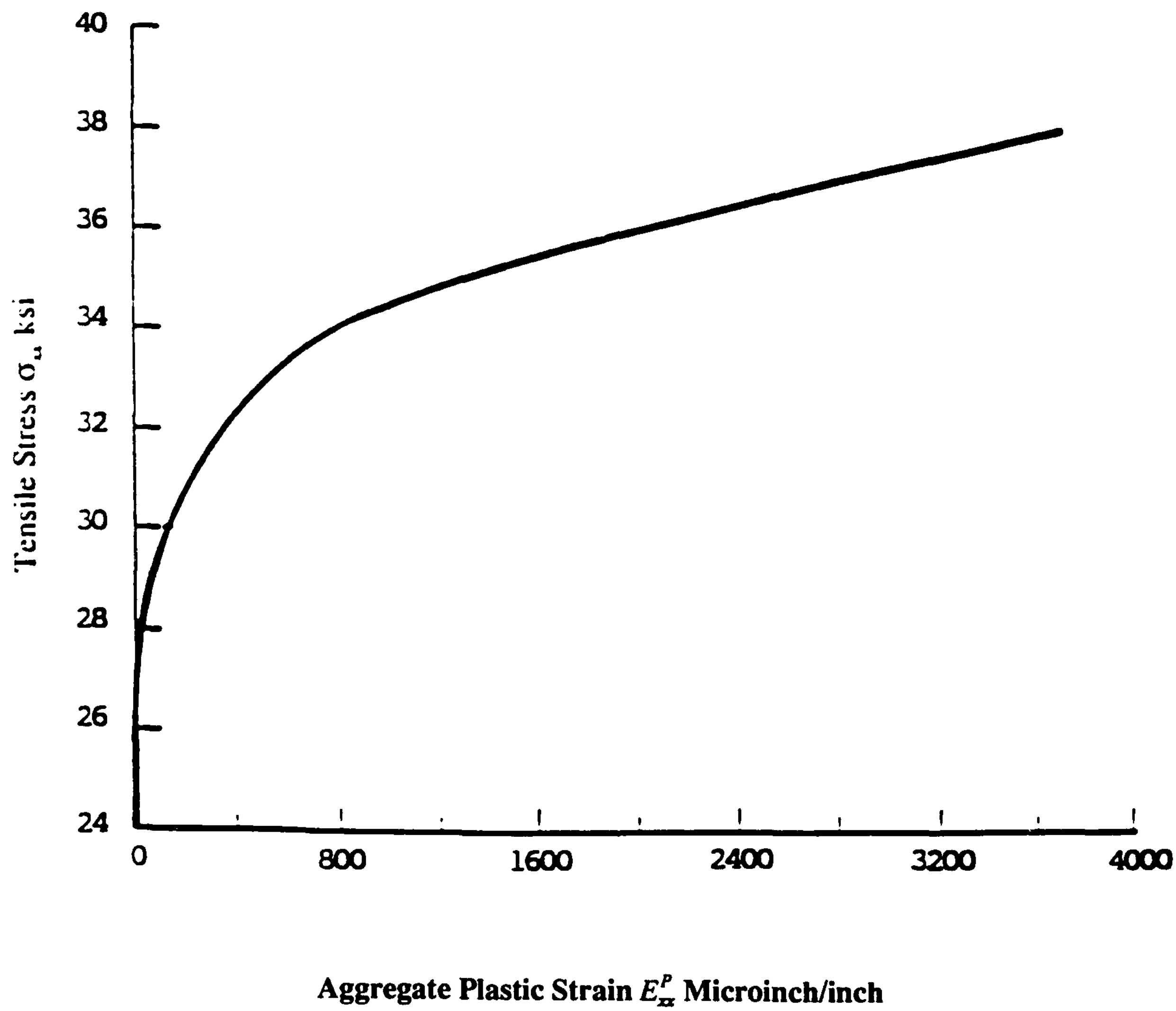


Fig. 7. Polycrystal 14ST A1.A1. Stress-Plastic Strain Curve in Uniaxial Tension

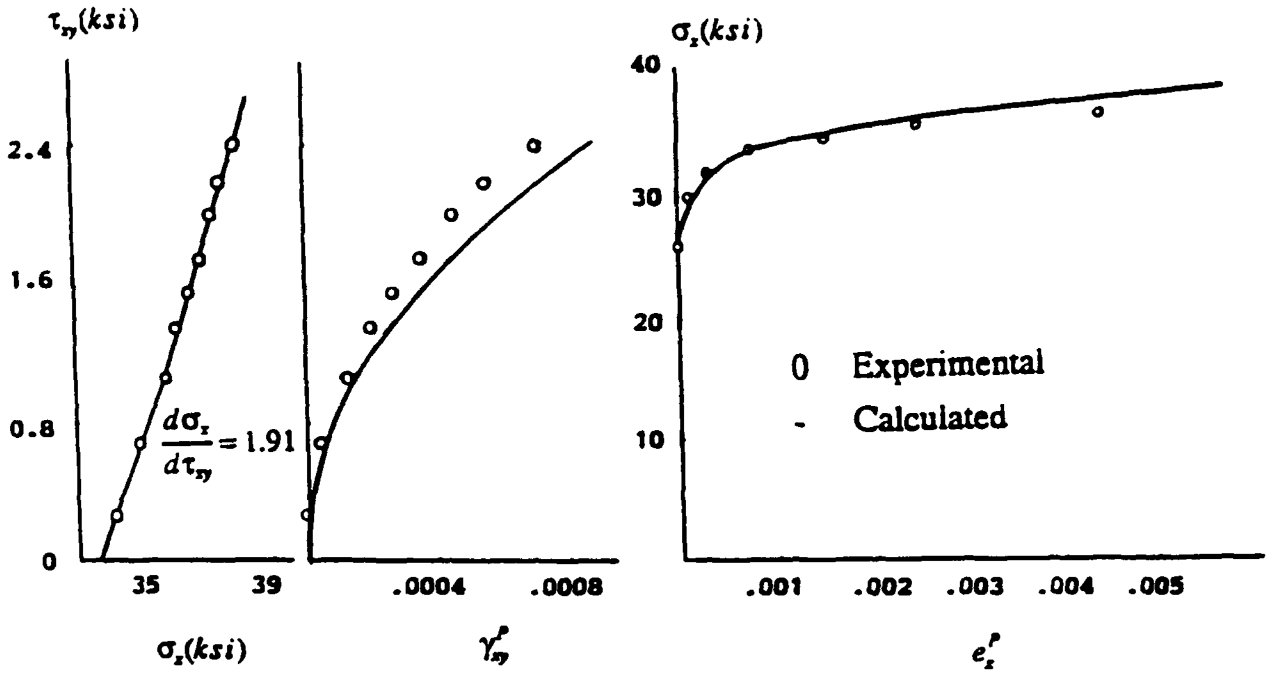


Fig. 8. Loading Path and Plastic Strains; $\frac{d\sigma}{d\tau} = 1.91$

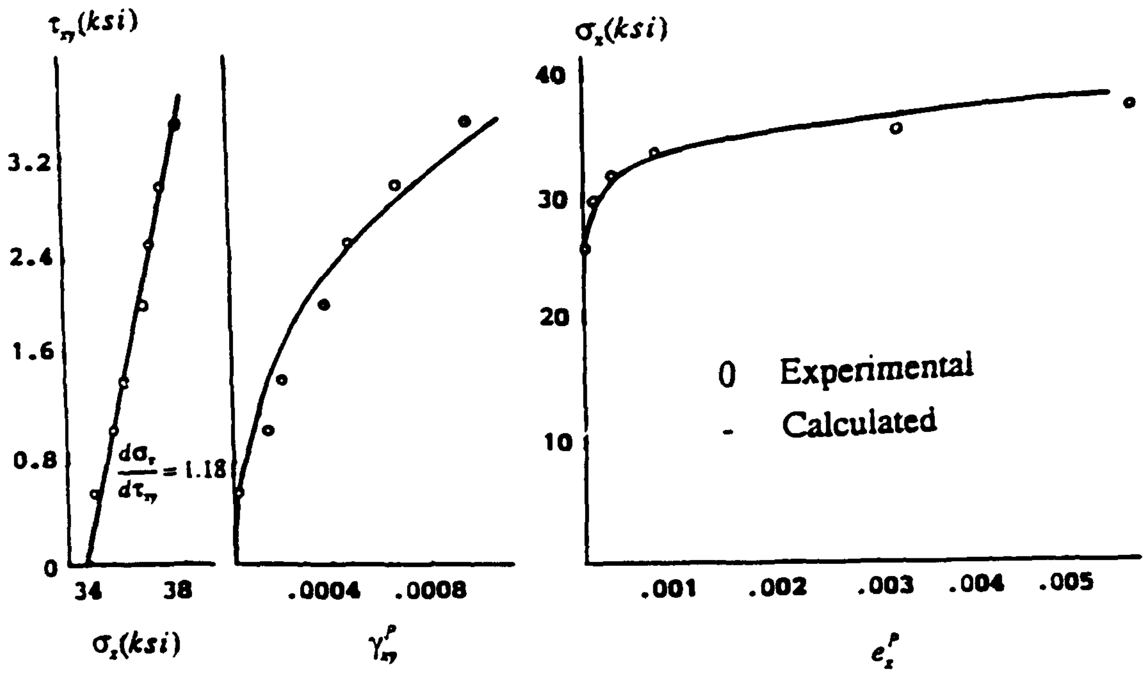


Fig. 9. Loading Path and Plastic Strains; $\frac{d\sigma}{d\tau} = 1.18$

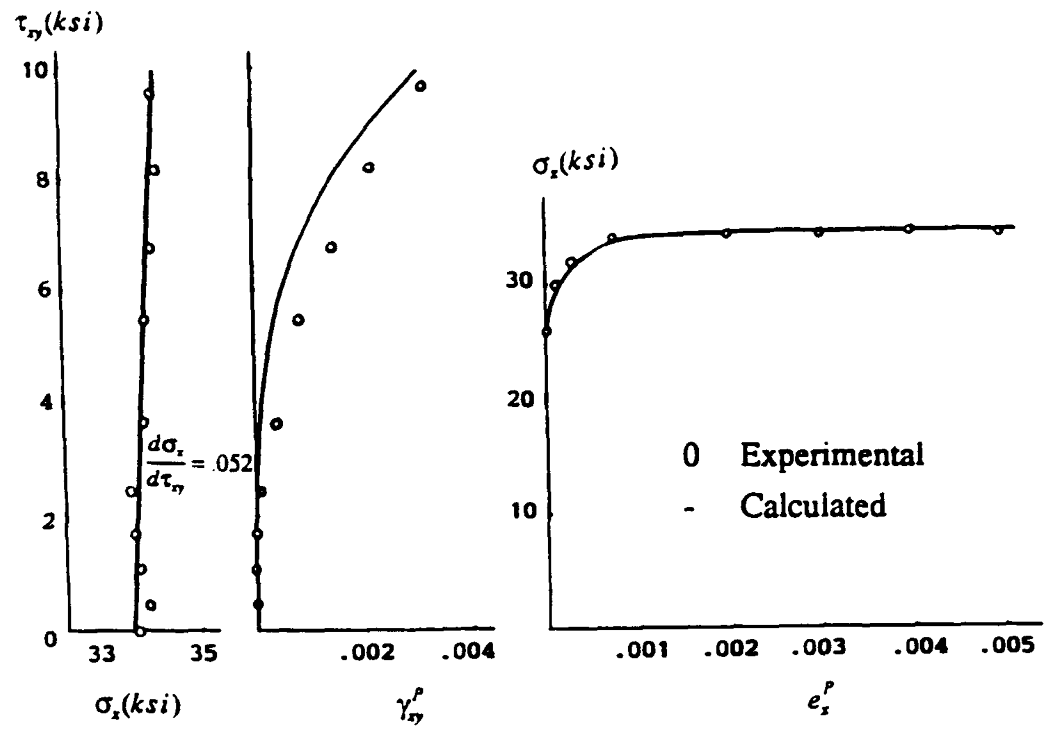


Fig. 10. Loading Path and Plastic Strains; $\frac{d\sigma}{d\tau} = 0.052$

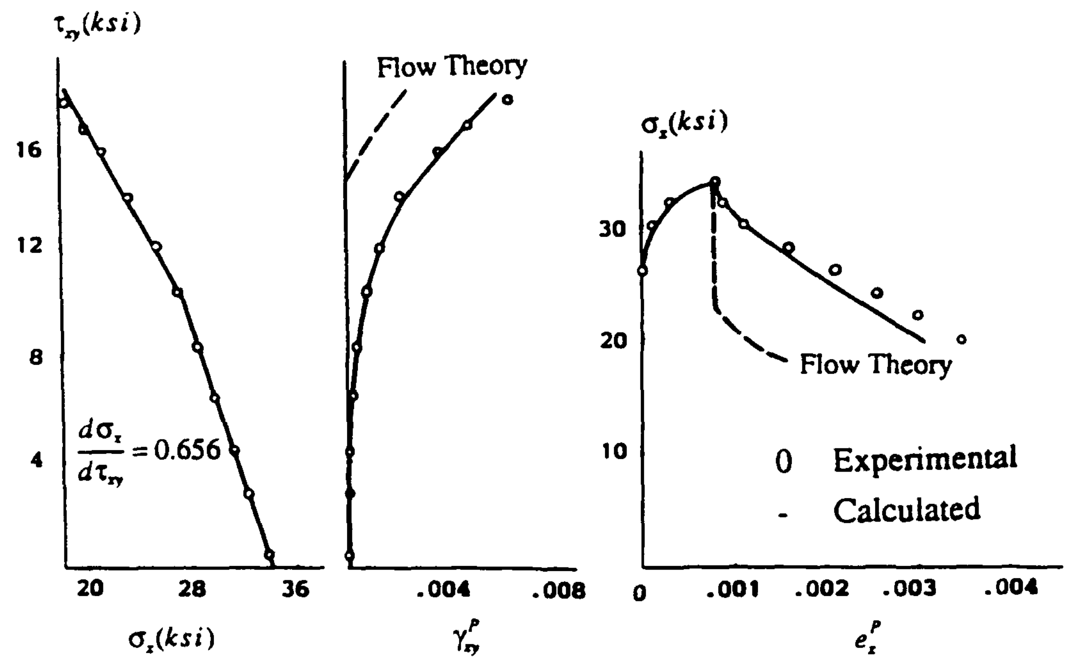


Fig. 11. Loading Path and Plastic Strains; $\frac{d\sigma}{d\tau} = -.656$

VI. Stress-Strain-Time Relationship

A. Mechanical Equation of State

Most structures are subject to stress varying with time. Creep tests have generally been done under constant stress. In applying these data to structures in which stress varies with time, certain assumptions have to be made. One commonly used assumption for creep analysis of structures is the existence of a mechanical equation of state between creep rate, stress, temperature, and current creep strain. The Mechanical Equation of State is not derived from the physics and therefore may not be valid for some metals. Under constant temperature, this equation may be written for a polycrystal,

$$\dot{E}^c_{11} = F(E^c_{11}, T_{11}) \tag{31}$$

where T_{11} is the macroscopic stress and F denotes a function. Here the stress is assumed to depend only on the current creep strain and its rate, and not on the strain rate during earlier stages of deformation. The creep behavior of the component crystal is generally assumed of similar form

$$\dot{\gamma}^c = F(\gamma^c, \tau) \tag{32}$$

Here τ represents the resolved shear stress, γ and $\dot{\gamma}$ denote the creep strain and creep strain rate, respectively in a slip system. It is interesting to find out whether this component crystal creep behavior would yield a similar macroscopic behavior given by (31). The strain-time curve under a constant tensile $T_{11} = 2800$ k.s.i. and the stress-strain-time curve of a relaxation test with an initial loading of 30,000 k.s.i. were calculated with a component crystal following the mechanical equation of state given by Eq. 32. It was found that at the same creep strain and the same strain rate, the stresses in both cases are the same. Hence the mechanical equation of state is satisfied for the macroscopic creep behavior in tensile loading. This is expected to hold also for other radial loadings. It is also noticed that the resolved creep strain rates of all the component crystals are the same at the instant, at which the macroscopic creep strains and strain rates of the creep test (constant load)

and the relaxation test are the same. This indicates that the mechanical equation of state can predict the creep behavior of polycrystalline solids reasonably well for radial loadings, but not for non-radial loadings.

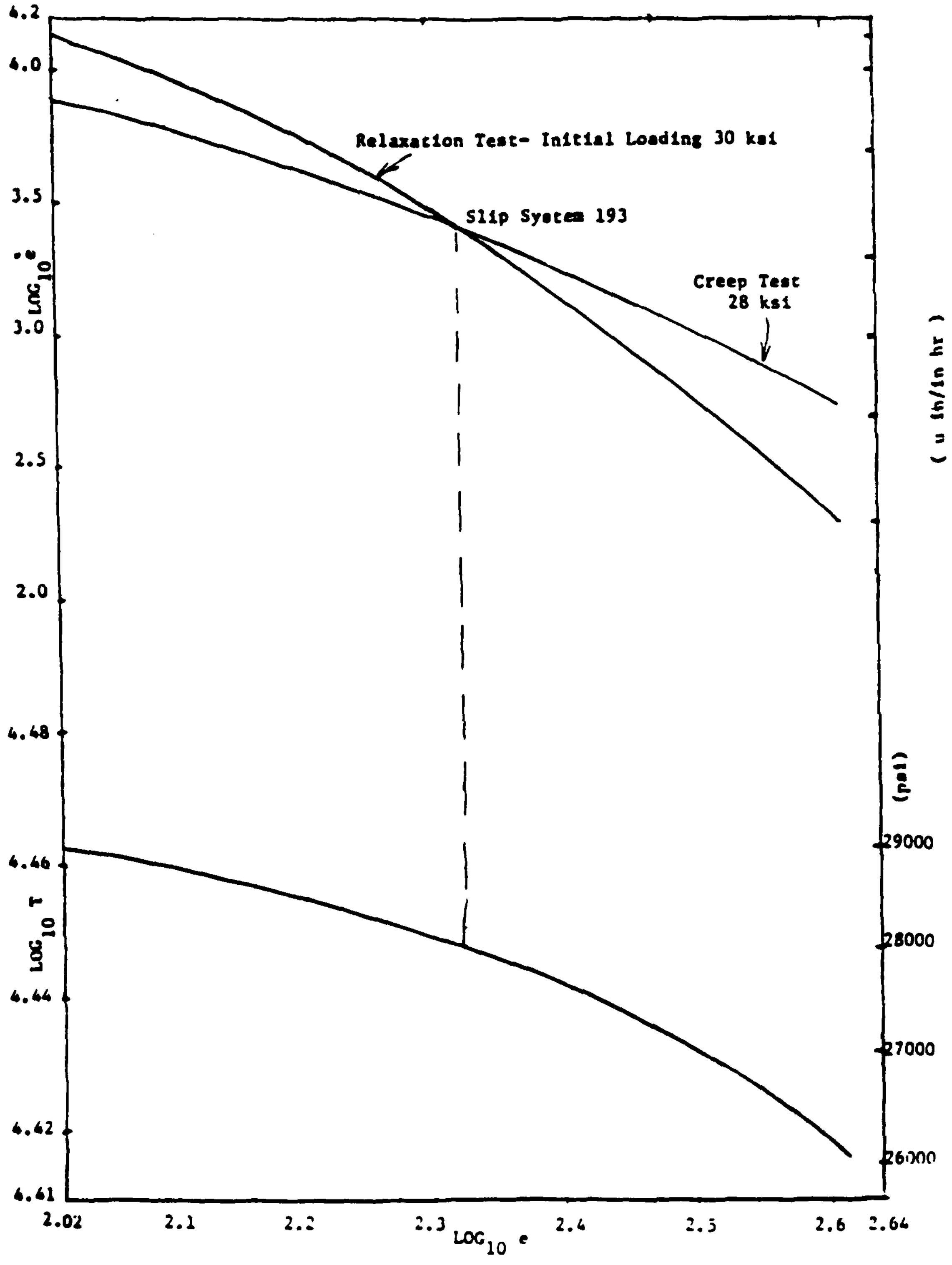


Fig. 12. Mechanical Equation of State Creep and Relaxation Behavior

B. Derivation of Component Crystal Stress-Strain-Time from Polycrystal Tests:

Component crystal creep behavior is expected to vary with grain size. Hence this crystal behavior is derived from polycrystal tests. It was informed by Prof. D.L. Ding that his test data by Ding and Lee published in *Proc. Exp. Mechanics*, Vol. 28, No. 3, p. 304, 1988 were performed from specimens of the same batch of materials and specimens of other tests might be obtained from different batches. Hence, the present development of micromechanic theory is based on this set of creep tests. In this development, the component crystal stress-strain-time relation is assumed to follow the mechanical equation of state. The slip rate in the *m*th slip system $\dot{\gamma}_m^c$ is assumed to depend on its resolved shear stress τ_m and slips in all the remaining slip systems. This is expressed as

$$\dot{\gamma}_m^c = f(\tau_m, \gamma_n^c\text{'s}) \tag{33}$$

where the superscript c denotes creep, the three sets of creep test data are shown in Figs. 13-15. A form of this component crystal creep satisfying the general mechanical equation of states as given in Eq. 33 has been found to represent the test data. Considering the creep to compose of the transient creep and steady creep. The creep rates are then

$$\dot{\gamma}_m^c = \dot{\gamma}_m^s + \dot{\gamma}_m^t \tag{34}$$

where

$$\dot{\gamma}_m^s = Cf(\tau_m, \gamma_n) \quad ;$$

$$\dot{\gamma}_m^t = Pf(\tau_m, \gamma_n)\varepsilon^{\left(-\frac{\gamma^t}{Q(\tau_m, \gamma_n)}\right)},$$

$$f(\tau_m, \gamma_n) = \left(\frac{\tau_m}{\tau_0}\right)^n \left[1 + R\left(\sum_{i \Sigma M} \gamma_i\right)^{\frac{1}{4}}\right],$$

and ε is the base of the natural logarithm.

M denotes the currently non-active slip systems. τ_0 is 10,000 p.s.i. C, P, Q, R and n are constants. They were found from the test data shown in Fig. 13,

$$
\begin{aligned}
C &= 0.48 \times 10^{-4} \\
P &= 70.0 \times 10^{-4} \\
Q &= 0.60 \times 10^{-4} \\
R &= 3.0 \\
n &= 6.0
\end{aligned}
$$

When there is a reduction of the resolved shear stress as shown in Fig. 16, ($\tau_{m_1} > \tau_{m_2}$), the recovery creep rate in this slp sysem, is represented by

$$\dot{\gamma}_m^R = f_R(\tau_m^R, \gamma_n)\left[C + P\varepsilon^{-\frac{\gamma_m^c}{\varpi_R\left(\tau_m^R, \gamma_n\right)}}\right] \tag{35}$$

where

$$
\begin{aligned}
f_R(\tau_m^R, \gamma_n) &= \left(\frac{\tau_m^R}{\tau_0}\right)^{n_R}\left[1 + R\left(\sum_{i \Sigma M} \gamma_i\right)^{\frac{1}{4}}\right] \\
\tau_m^R &= \alpha(\tau_{m_1} - \tau_{m_2}), \qquad \alpha = \frac{1}{2} \\
n_R &= 3.5
\end{aligned}
$$

The above expressions were used to calculate the stress-strain-time curves of the tests shown in Figs. 15 & 16. The corresponding curves calculated by Von Mise's criterion are also shown in the same figures (14 to 16). It is seen that the present theory represents the test data much better than the Von Mise's theory.

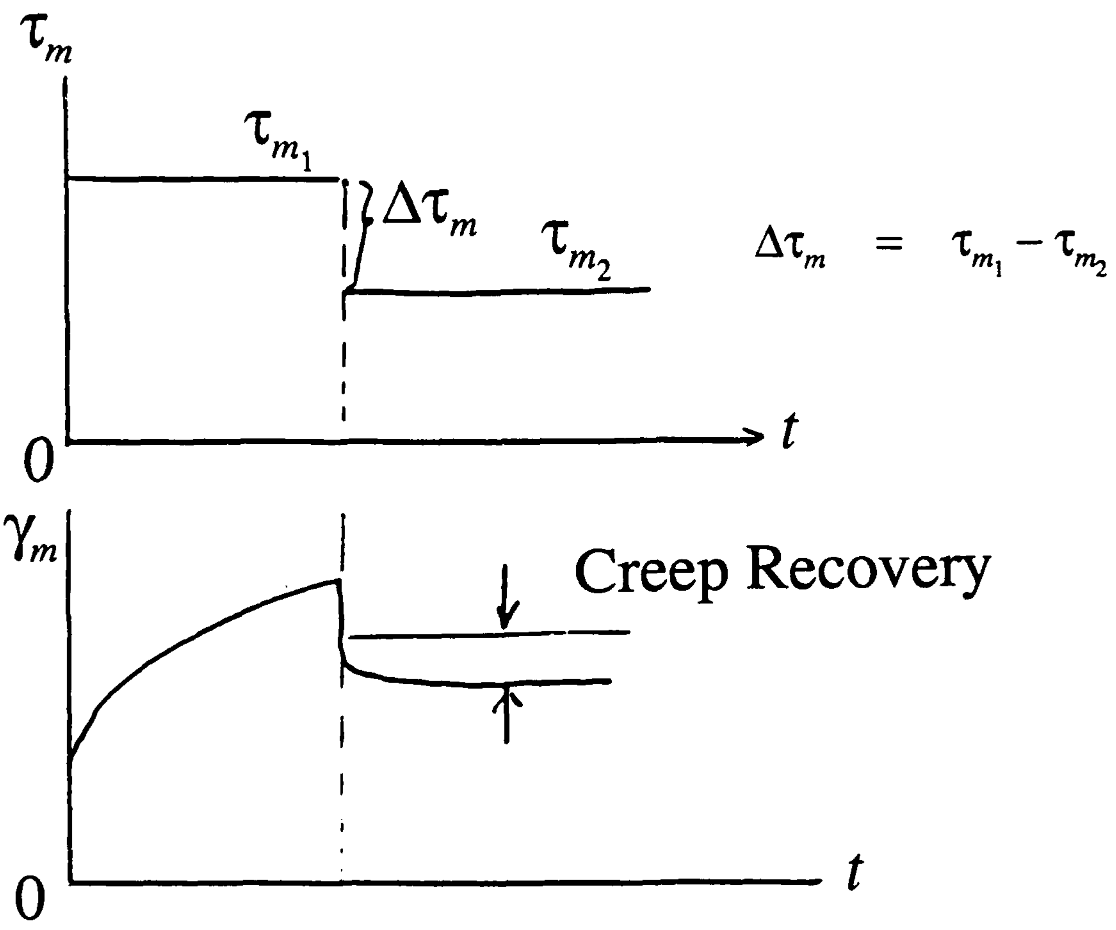
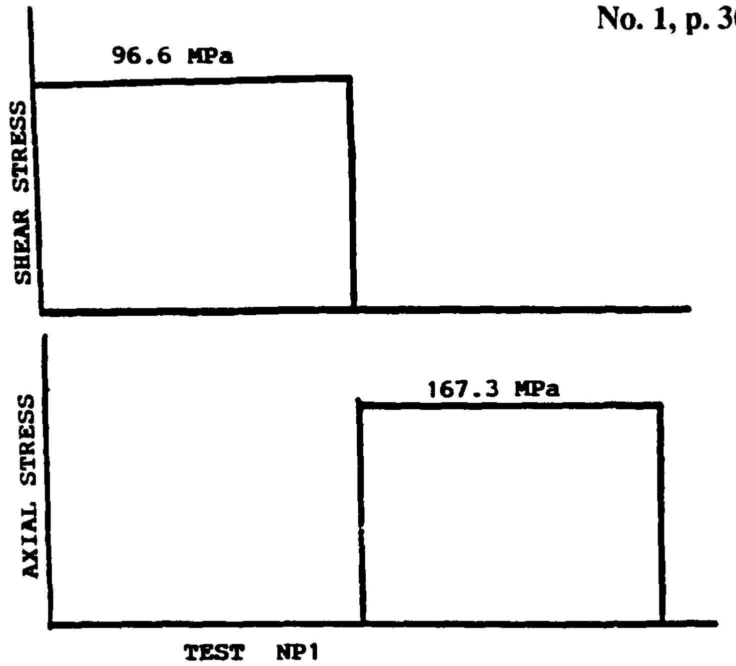


Fig. 13. Creep Recovery

Fig. 14. Calculated vs Experimental Creep Strain under Non-Radial Loadings - Test Data Specimen No. 1

by Ding & Lee (Exp. Mech. Vol. 28, No. 1, p. 304-309, 1988)



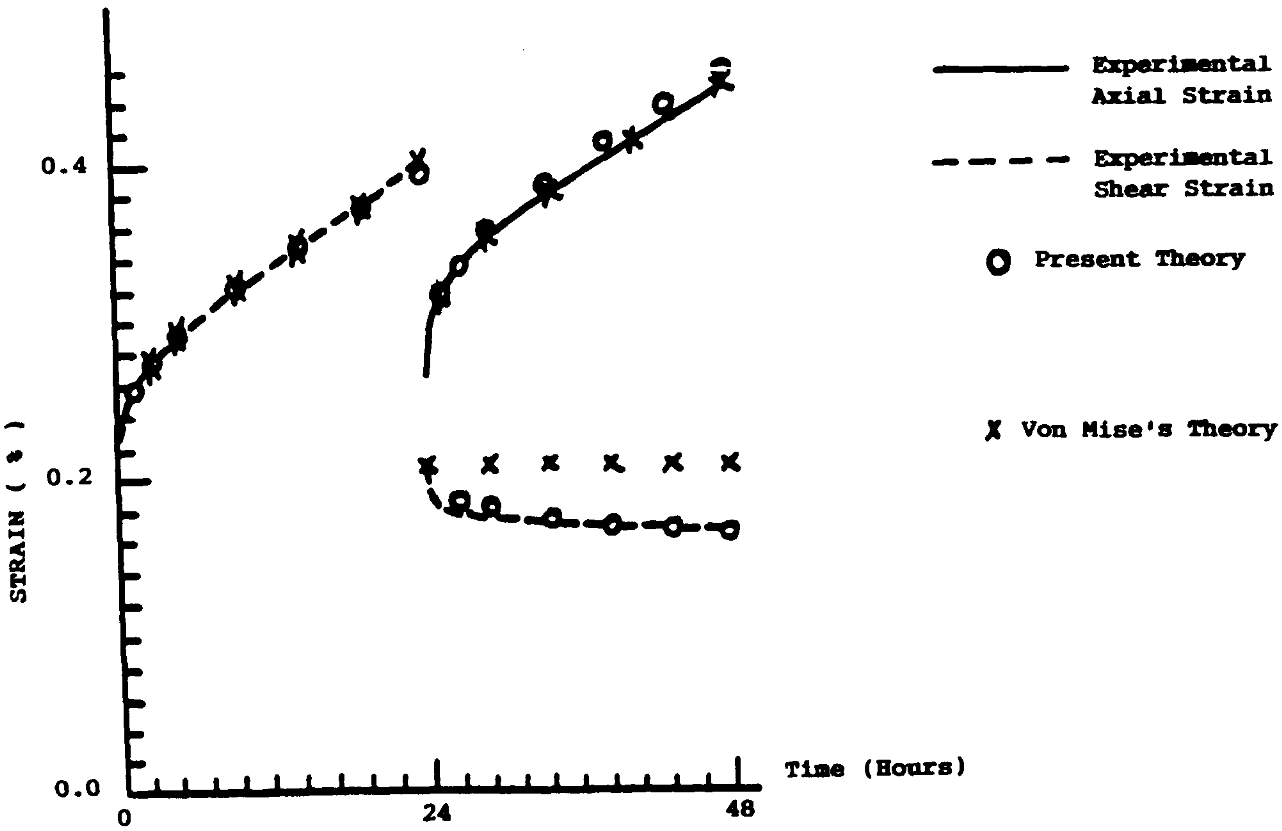


Fig. 15. Calculated vs Experimental Creep Strain under a Non-Radial Loading. Specimen No. 2

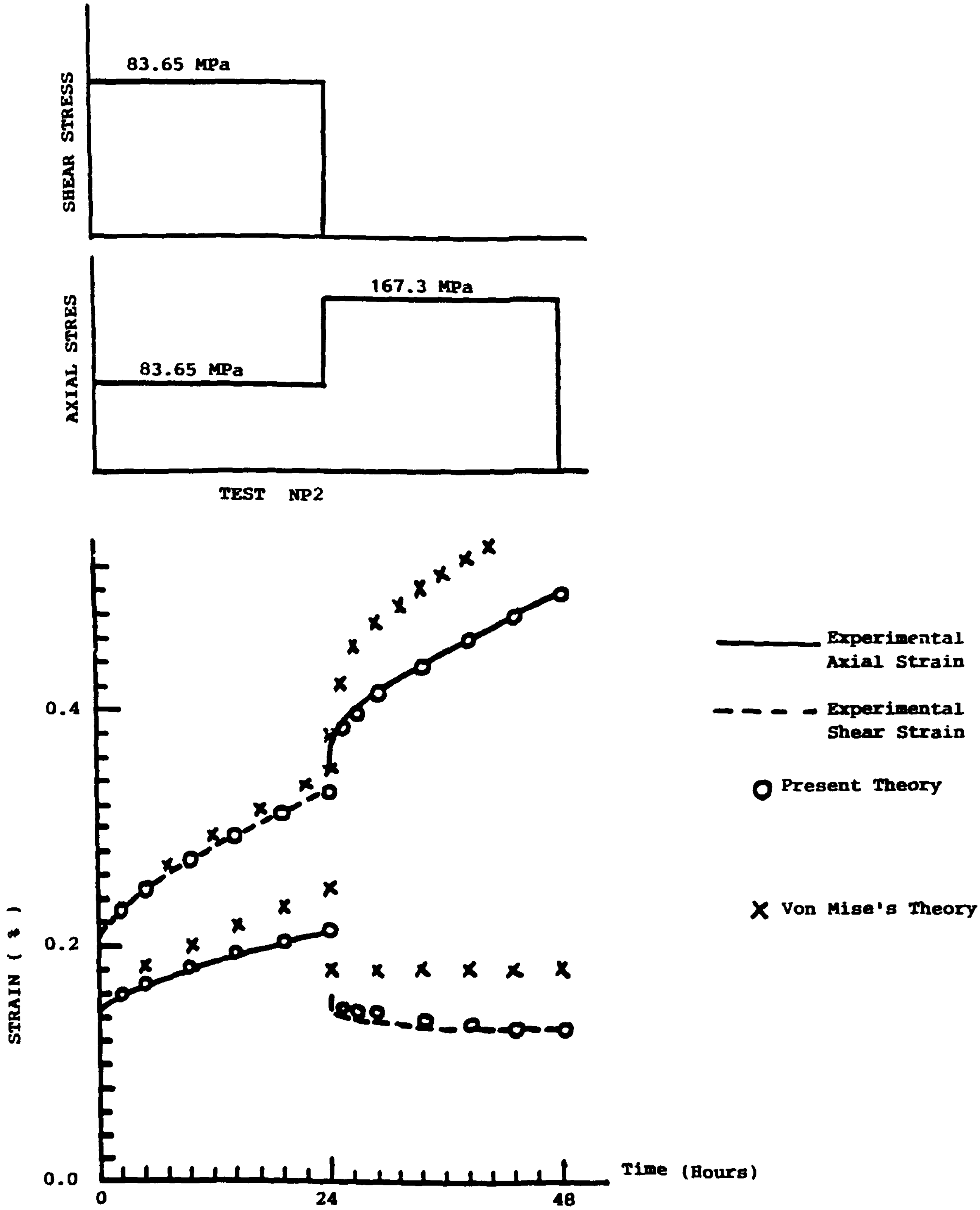
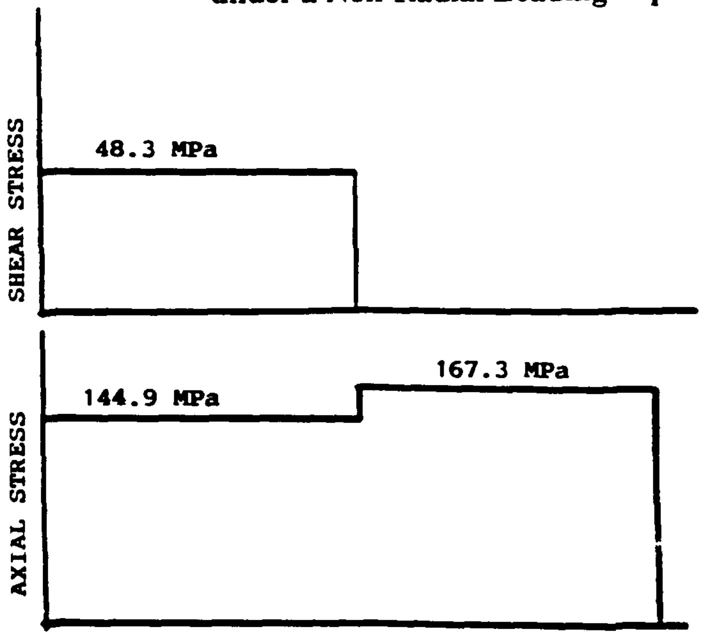
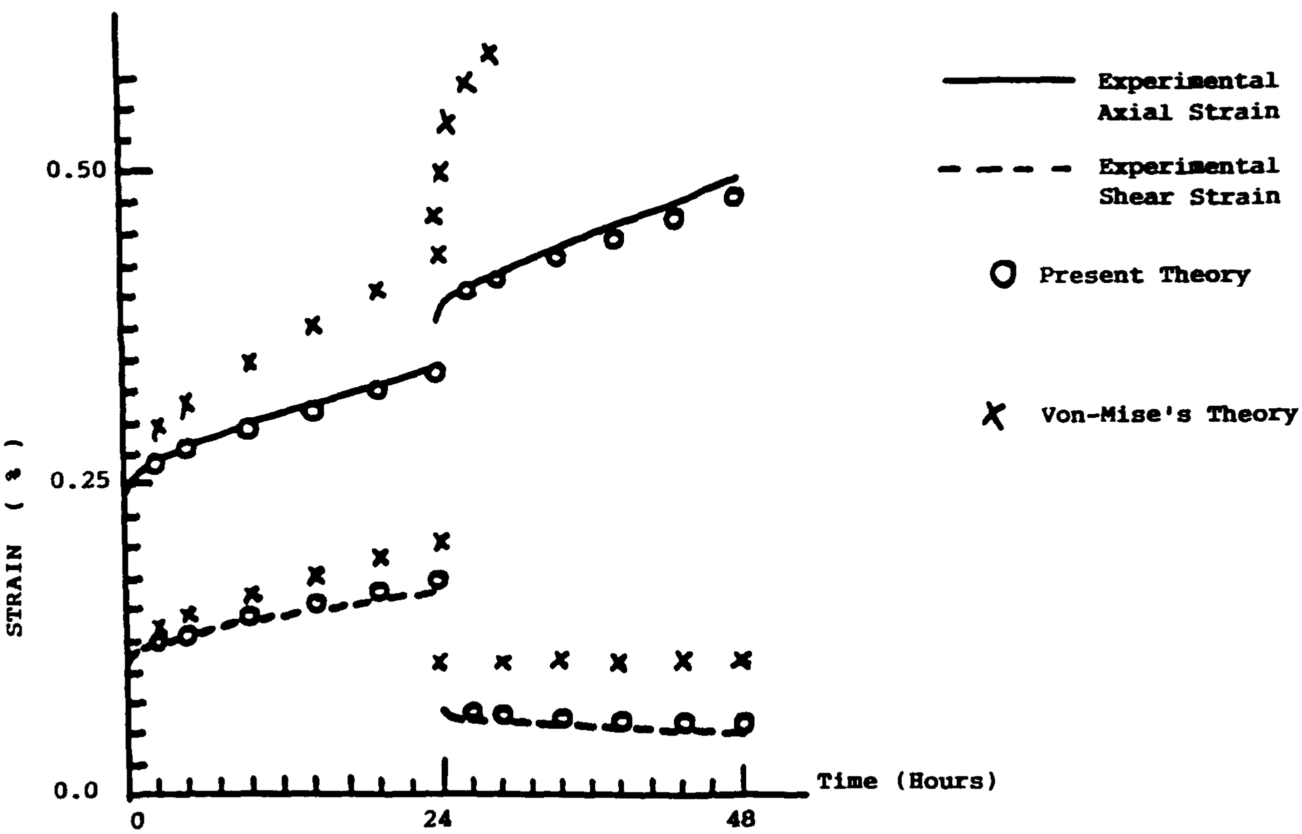


Fig. 16. Calculated vs Experimental Creep Strain under a Non-Radial Loading. Specimen No. 3



TEST NP3



VII. Conclusions

The derivation of the polycrystal stress-strain and the stress-strain-time relation from those of the component crystal satisfies both the equilibrium and compatibility conditions and hence fulfills all the requirements of continuum mechanics. The calculation of component crystal deformation behavior (both time-independent and time dependent) from polycrystal test data automatically takes care of the crystal size effect on the plastic deformation. Refined single crystal data obtainea by Bassani, 1990 and Wu et al., 1990, including those with change of crystal orientations are embodied in the representation of the component crystal characteristics. More such data are dsirable. Their interpretation of the single crystal data contributes greatly to the development of this plasticity theory. Component crystal characteristics, previously derived from polycrystal tensile test data, are presently derived from both polycrystal tensile and non-radial loadings. The calculated incremental stress-strain results are compared with the experiments. The agreement is seen to be quite good. This will increase the accuracy of elastic-plastic analyses and designs of many structures.

A micromechanic theory of creep in polycrystalline solids is also developed. We have learned that creep test data under non-radial loading given by Ding and Lee 1988 were performed on test specimens from the same batch of material and other test data may not be from the same batch. Hence Ding and Lee's data were used for the development of the present theory. The slip rate of a slip system of the component crystal is assumed to be a function of the resolved shear stress of the system and the amounts of slip in all slip systems. A form of this function to satisfy a non-radial loading was found. This function was used to calculate the stress-strain-time relations of two other non-radial loadings. Similar calculations were made using Von Mise's criterion for plasticity. These calculated results were shown in Figs. 14 to 16. It is seen from these figures, the present theory agrees well with the experimental data. Von Mise's model deviate considerably from the test data.

These developed methods should be able to improve the accuracy of the analyses and design of many structures.

During the course of this research, one graduate student X.Q. Wu supported by the grant has received his Ph.D. degree, students Qiye Chen and Wei Zhong, supported by this grant have received their M.S. degrees.

VIII. Acknowledgement

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